Coarse-graining of many-particle stochastic systems: mathematical and numerical methods.

Petr Plecháč *

Abstract: In this contribution we present results of the recent work on coarse-graining methods for microscopic stochastic lattice systems. We emphasize the numerical analysis of the schemes, focusing on error quantification as well as on the construction of improved algorithms capable of operating in wider parameter regimes. We also discuss adaptive coarse-graining schemes which have the capacity of automatically adjusting during the simulation if substantial deviations are detected in a suitable error indicator. The methods employed in the development and the analysis of the algorithms rely on a combination of statistical mechanics methods (renormalization and cluster expansions), statistical tools (reconstruction and importance sampling) and PDE-inspired analysis (*a posteriori* estimates). We also discuss the connections and extensions of our work on lattice systems to the coarse-graining of polymers.

On specific examples of lattice as well as off-lattice dynamics (simulations of spin systems or polymers) we demonstrate that computational implementation of constructed hierarchical algorithms leads to significant speed up of simulations. Results from the joint work with M. A. Katsoulakis and L. Rey-Bellet (University of Massachusetts) will be presented.

*Deaprtment of Mathematics, University of Tennessee and Oak Ridge National Laboratory.